Claims

1. A method for searching stable docking models of biopolymer-ligand molecule complex, which comprises the steps of: (1) searching possible hydrogen-bond schemes between a biopolymer and a ligand molecule by preparing possible combination sets of hydrogen-bonding heteroatoms in the ligand molecule with dummy atoms located at the positions of heteroatoms that can be hydrogen-bond partners to hydrogen-bonding functional groups in the biopolymer; (2) estimating the possible the hydrogen-bond schemes between the biopolymer and ligand molecule and the possible conformations of a hydrogen-bonding part of the ligand molecule at the same time by comparing the distances between the dummy atoms with the distances between the hydrogen-bonding heteroatoms; and (3) obtaining the possible docking models of the biopolymer-ligand molecule complex by changing the coordinates of all atoms of the ligand molecule into the coordinate system of the biopolymer, according to the correspondences between the hydrogen-bonding heteroatoms in the ligand molecule and the dummy atoms in combination sets for each of the hydrogen-bond schemes and conformations obtained in the second step.

2. A method for searching stable docking models of biopolymer-ligand molecule complex, which comprises the steps of: (1) searching possible hydrogen-bond schemes between a biopolymer and a ligand molecule by preparing possible combination sets of hydrogen-bonding heteroatoms in a partial structure of the ligand molecule and dummy atoms located at the positions of heteroatoms that can be hydrogen-bond partners to hydrogen-bonding functional groups in the biopolymer; (2) estimating the possible hydrogen-bond schemes between the biopolymer and ligand molecule and the possible conformations of the partial structure in the ligand molecule at the same time by comparing the distances between the

dummy atoms with the distances between the hydrogen-bonding heteroatoms; (3) specifying on the basis of the hydrogen-bond schemes and conformations obtained in the second step, those combination sets of the hydrogen-bonding heteroatoms and dummy atoms which provide hydrogen-bond schemes that are impossible in the partial structure of the ligand molecule, and hydrogen-bonding heteroatoms that cannot form any hydrogen-bond with the dummy atoms; (4) searching possible hydrogen-bond schemes between the biopolymer and the whole ligand molecule by preparing possible combination sets of the dummy atoms and the hydrogen-bonding heteroatoms in the whole ligand molecule excluding the combination sets containing the hydrogen-bonding heteroatoms specified in the third step and the combination sets of the dummy atoms and hydrogen-bonding heteroatoms that are specified in the third step; (5) estimating the hydrogen-bonding schemes between the biopolymer and ligand molecule and the conformations of a hydrogen-bonding part of the ligand molecule at the same time by comparing the distances between the dummy atoms with the distances between the hydrogen-bonding heteroatoms in the ligand molecules; and (6) obtaining possible docking models of the biopolymer-ligand molecule complex by changing the coordinates of all atoms of the ligand molecule into the coordinate system of the biopolymer, according to the correspondences between the hydrogen-bonding heteroatoms in the ligand molecule and the dummy atoms in combination sets for each of the hydrogen-bond schemes and conformations obtained in the fifth step.

3. A method for searching stable docking models of biopolymer-ligand molecule complex, which comprises the steps of: (1) searching possible hydrogen-bond schemes between a biopolymer and a ligand molecule by preparing possible combination sets of hydrogen-bonding heteroatoms in

the ligand molecule with dummy atoms located at the positions of heteroatoms that can be hydrogen-bond partners to hydrogen-bonding functional groups in the biopolymer; (2) estimating the possible hydrogen-bond schemes between the biopolymer and ligand molecule and the possible conformations of a hydrogen-bonding part of the ligand molecule at the same time by comparing the distances between the dummy atoms with the distances between the hydrogen-bonding heteroatoms; and (3) optimizing the conformations of the ligand molecule in such a manner that the positions of the dummy atoms will coincide with the positions of the hydrogen-bonding heteroatoms in the ligand molecule while retaining the hydrogen-bond schemes obtained in the second step and thereafter excluding the conformations of the ligand molecule with intramolecular energies higher than given values; (4) obtaining possible docking models of the biopolymer-ligand molecule complex by changing the coordinates of all atoms of the ligand molecule into the coordinate system of the biopolymer according to the correspondences between the hydrogen-bonding heteroatoms in the ligand molecule and the dummy atoms in combination sets for each of the conformations that have not been excluded in the third step; (5) excluding the docking models of the hydrogen-bonding part of the ligand molecule with intramolecular energies higher than given values or the intermolecular interaction energies higher than given values between the biopolymer and the hydrogen-bonding part of the ligand molecule, and thereafter optimizing the docking models unexcluded; (6) generating the conformations of a non-hydrogen-bonding part of the ligand molecule for each of the docking models obtained in the fifth step, thereby obtaining new docking models; and (7) excluding the docking models of the whole ligand molecule with intramolecular energies higher than given values and the

intermolecular interaction energies higher than given values between the biopolymer and the whole ligand molecule, and thereafter optimizing the complex structures unexcluded.